Final Report

"Characterization of Boron Atom Aggregation"
SPC 01-4069: contract order number F61775-01-WE069

This special contract was awarded $20,000 for a year's support for the project investigating the electronic spectra of boron clusters and their aggregation in neon matrices. It was designated as a follow up to the proposal (SPC 00-4073) and was carried out in the period 1.April 2001 to 31.March 2002. Involved in this investigation was the experimental group of the principal investigator- Prof.J.P.Maier at the Institute of Physical Chemistry, University of Basel, Switzerland, as well as the theoretical groups of Prof.P.Rosmus, Theoretical Chemistry, University of Marne-la-Vallee, France and of Prof.W.Meyer, Theoretical Chemistry, University of Kaiserslautern, Germany. Throughout the project, exchange of information was maintained with Dr.C.W.Larson, Air Force Research Laboratory, Edwards AFB. Evgueni Riaplov was the PhD student in Basel who carried out the experimental studies.

Following the initial success as part of the preceeding proposal in observing for first time the electronic absorption spectra of B_3 and B_3^- in 5K neon matrices, a number of experiments were undertaken in Basel and theoretical calculations by the groups of Rosmus and Meyer in order to understand the details of the complex vibronic structure in the spectra. Spectra with improved S/N for B_3 and B_3^- were obtained. This involved primarily optimization of the cesium sputter source for the production of the B_3^- ion beam for the mass-selected codeposition with excess of neon. The experiment uses the special apparatus developed in Basel which combines mass-selection with matrix isolation spectroscopy.

A number experiments were undertaken during the course of the year's project, primarily aimed at trying to observe the electronic spectra of the next larger boron species, B_4. These were unsuccessful because we could not obtain sufficient current of B_4^- from the ion source. For this purpose both a B_4C rod and LaB_6 rods were used; the mass-spectral pattern obtained as result of the cesium sputtering were similar and an example is shown in the figure below. (The BO^- species arises from the presence of CsO in the source).

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (FROM - TO)
02-04-2002	Final rept.	01-04-2001 to 01-04-2002

4. TITLE AND SUBTITLE
Characterization of Boron Atom Aggregation
Unclassified

5a. CONTRACT NUMBER
F61775-01-WF069

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Maier, John P. ;

5d. PROJECT NUMBER

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME AND ADDRESS
University of Basel
Klingelbergstrasse 80
Basel CH-4056, Switzerlandxxxxx

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME AND ADDRESS
EOARD
PSC 802 Box 14
FPO, xx09499-0014

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
APUBLIC RELEASE
,

13. SUPPLEMENTARY NOTES

14. ABSTRACT

This report results from a contract tasking University of Basel as follows: The contractor will investigate and understand the electronic spectra of matrix isolated B, B2, B3 and higher clusters and to apply these understandings in quantitative analysis of B atom reactions in rare gas cryogenic solids. A number of experiments were undertaken and theoretical calculations in order to understand the details of the complex vibronic structure in the electronic absorption spectra of B3 and B3 - in 5K neon matrices. Spectra with improved S/N for B3 and B3 - were obtained. A number experiments were undertaken aimed at trying to observe the electronic spectra of the next larger boron species, B4. These were unsuccessful because we could not obtain sufficient current of B4 - from the ion source. Concurrent to the experimental studies, extensive theoretical studies of B3 were undertaken to understand the complex vibronic structure observed in the electronic spectrum as result of Jahn-Teller effects.

15. SUBJECT TERMS
EOARD; Propellants; high energy density matter

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE	Public Release	6	Fenster, Lynn lfenster@dtic.mil
Unclassified	Unclassified	Unclassified			19b. TELEPHONE NUMBER International Area Code Area Code Telephone Number 703767-9007 DSN 427-9007

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From – To)*
02-04-2002	Final Report	01 April 2001 - 01-April-02

4. TITLE AND SUBTITLE

Characterization of Boron Atom Aggregation

5a. CONTRACT NUMBER
F61775-01-WE069

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)

Professor John P Maier

5d. PROJECT NUMBER

5d. TASK NUMBER

5e. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Basel
Klingelbergstrasse 80
Basel CH-4056
Switzerland

8. PERFORMING ORGANIZATION REPORT NUMBER

N/A

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

EOARD
PSC 802 BOX 14
FPO 09499-0014

10. SPONSOR/MONITOR'S ACRONYM(S)
EOARD

11. SPONSOR/MONITOR'S REPORT NUMBER(S)
SPC 01-4069

12. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

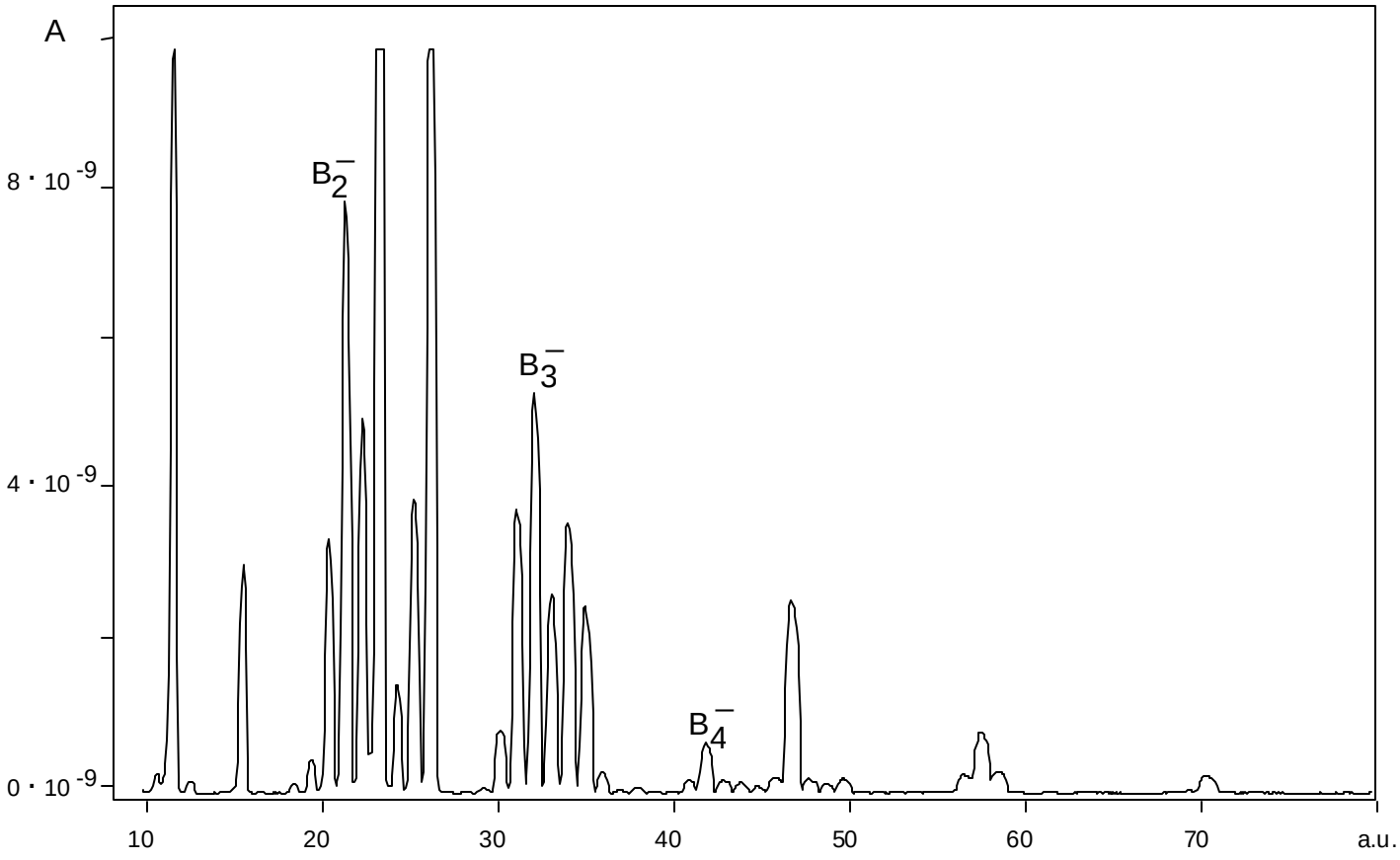
13. SUPPLEMENTARY NOTES

14. ABSTRACT

This report results from a contract tasking University of Basel as follows: The contractor will investigate and understand the electronic spectra of matrix isolated B, B2, B3 and higher clusters and to apply these understandings in quantitative analysis of B atom reactions in rare gas cryogenic solids. A number of experiments were undertaken and theoretical calculations in order to understand the details of the complex vibronic structure in the electronic absorption spectra of B_3 and B_3^- in 5K neon matrices. Spectra with improved S/N for B_3 and B_3^- were obtained. A number experiments were undertaken aimed at trying to observe the electronic spectra of the next larger boron species, B_4. These were unsuccessful because we could not obtain sufficient current of B_4^- from the ion source. Concurrent to the experimental studies, extensive theoretical studies of B_3 were undertaken to understand the complex vibronic structure observed in the electronic spectrum as result of Jahn-Teller effects.

15. SUBJECT TERMS
EOARD, Propellants, high energy density matter

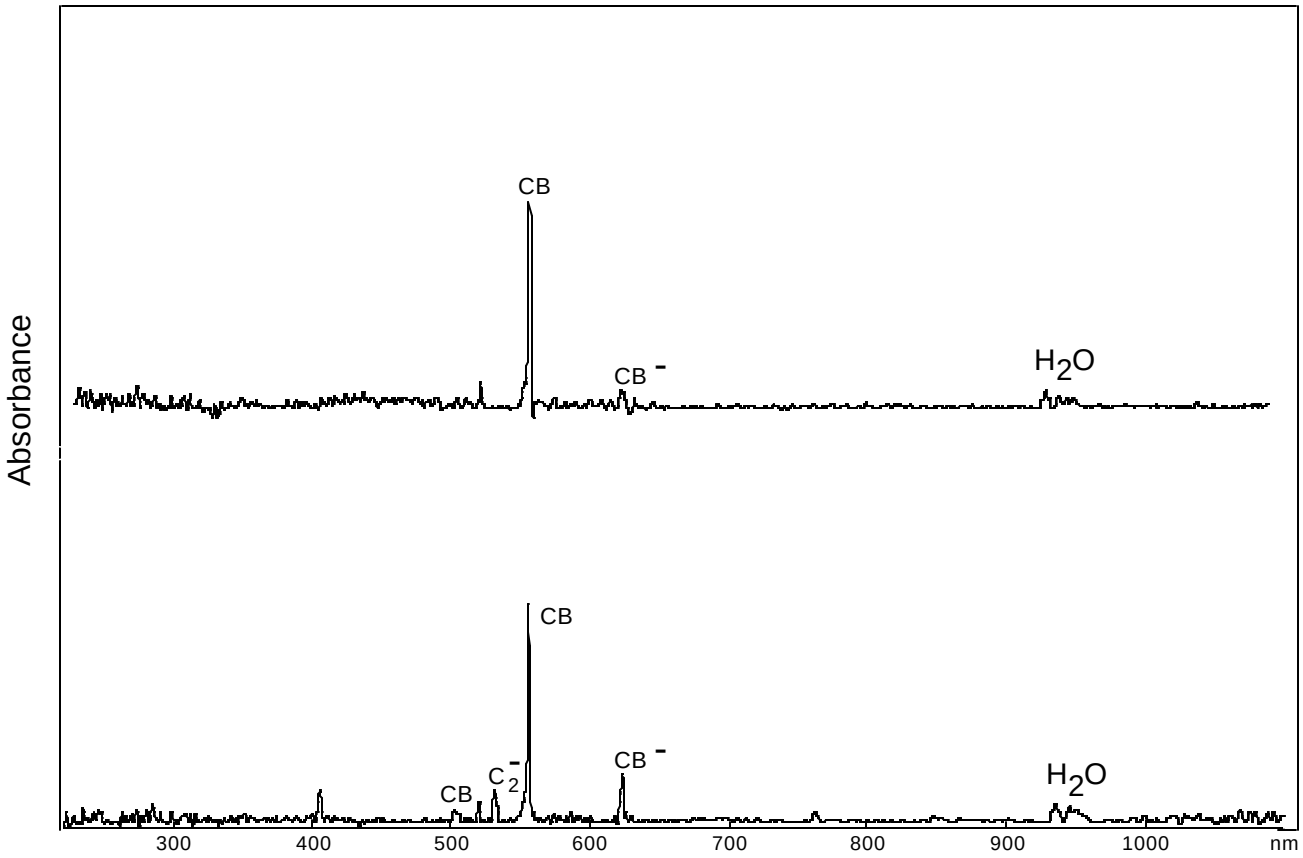
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18, NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Ingrid Wysong
UNCLAS	UNCLAS	UNCLAS	UL	5	19b. TELEPHONE NUMBER *(Include area code)* +44 (0)20 7514 4285



Whereas the best current achieved for B_4^- was 0.5 nA with the B_4C rod, it was a factor of ten less with LaB_6. In order to be able to record the spectra in the future a source which will produce an order of magnitude larger current for the mass-selected species needs to be found.

Attempts to produce larger boron species by aggregation were also undertaken. In this mass-selected B_2^- (about 20 nA current) was codeposited with argon to produce a matrix at around 12 K. The neutral B_2 was produced by irradiation during or after deposition. The matrix was then annealed to 28 K. However, no new absorptions apart that of B_2 could be observed. This is in contrast to the analogous experiments carried out earlier with C_2 where numerous longer carbon chains could be identified. The difference is attributed to the much smaller concentrations achieved with boron as opposed to carbon; the mass-selected current was several orders of magnitude larger in the latter case.

In another set of experiments, B_2C^- was codeposited with neon to try to observe this anion as well as its neutral counterpart. The results of such an measurement are illustrated by the figure below.



The bottom trace is the absorption spectrum observed after mass-selected deposition. New absorptions were not observed; only the known electronic systems of CB and CB^- (and of C_2^-) produced by fragmentation during matrix-growth (and the overtone vibrational transitions of water impurity). The top trace is the spectrum after the matrix is bleached by irradiation with 4.9 eV photons. As can be seen, the anion signals are either eliminated (C_2^-) or significantly reduced (BC^-) while the signal of CB growths.

Numerous related studies were carried out, depositing BH_2^- (4nA current) or CBO^- (2 nA) but no new species were detected, whereas deposition of BS_2^- or BO_2^- lead to the observation of the known electronic absorption spectra of BS_2, or BO_2 respectively. In the case of the latter species, the mass-selected experiment confirms the identification of this molecule after pure boron atom deposition (as reported in the final report SPC 00-4073) and its in situ formation in the matrix due to the presence of O_2 as impurity.

Concurrent to the experimental studies in Basel, extensive theoretical studies of B_3 were undertaken in collaboration with the groups of P.Rosmus and W.Meyer. Specifically the aim is to understand the complex vibronic structure observed in the electronic spectrum as result of Jahn-Teller effects. A Diploma work on this topic has been written by T.Weber, working under the guidance of W.Meyer (this can be supplied by request, though it is written in German). However Prof.W.Meyer is still not satified with the quality of the theory and as result the experimental data on B_3 and B_3^- remains unpublished.

(1) “The Contractor, Institute for Physical Chemistry, hereby declares that, to the best of its knowledge and belief, the technical data delivered herewidth under Contract Order Number F61775-01-WE069 is complete, accurate and complies with all the requirements of the contract.”

Date 27.March, 2002
Name and Title of Authorized official: John P.Maier, Professor, Director of Institute for Physical Chemistry

(2) (**B**) “I certify that there were no subject inventions to declare as defined in FAR 52.227-13, during the performance of this contract.”

Date 27.March, 2002
Name and Title of Authorized official: John P.Maier, Professor, Director of Institute for Physical Chemistry

Professor J.P.Maier
Institute for Physical Chemistry
University of Basel, Switzerland